The Quantum-Classical Transition in Nonlinear Dynamical Systems

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Viewed as approximations to quantum mechanics, classical evolutions can violate the positive-semidefiniteness of the density matrix. The nature of this violation suggests a classification of dynamical systems based on classical-quantum correspondence; we show that this can be used to identify when environmental interaction (decoherence) will be unsuccessful in inducing the quantum-classical transition. In particular, the late-time Wigner function can become positive without any corresponding approach to classical dynamics. In the light of these results, we emphasize key issues relevant for experiments studying the quantum-classical transition.

In recent years much effort has been expended, both theoretically and experimentally, to explore the transition from quantum to classical behavior in a controlled way. In this context, the interaction of trapped, cold atoms with optical potentials, both time-dependent and independent, has become a topic of considerable interest and activity [1,2]. The experimental ability to systematically study dissipative quantum dynamics of nonlinear systems is an exciting new area where the frontier between classical and quantum mechanics may be carefully examined.

In this Letter we wish to explore some of the key qualitative features of the quantum-classical transition. We establish that with $\hbar$ fixed at a finite value, and classical dynamical evolution equations for phase space distribution functions viewed as approximations to the underlying quantum equations, classical Liouville and Master equations violate the quantum constraint of positive-semidefiniteness of the density matrix: We refer to this property of the density matrix as 'rho-positivity'. There is thus a global obstruction to the classical limit arising directly from quantum evolutions. We argue below that rho-positivity violation can (1) serve as a guide in classifying dynamical systems with regard to classical-quantum correspondence: weak violation as Type I, strong violation as Type II, and (2) explain robustness to decoherence in the sense of avoidance of the classical limit as exemplified by dynamical localization in the (open-system) quantum delta kicked rotor (QDKR). Our results impact directly on the interpretation and design of experiments to test various aspects of the quantum-classical transition.

As described in more detail below, certain nonclassical aspects of the dynamics of the QDKR turn out to be stable to decohering effects of external noise and decoherence due to spontaneous emission. A dynamical description in terms of the Wigner function leads to two alternatives to explain this stability: (1) diffusion in the quantum Master equation is simply not efficient at suppressing quantum interference terms present in the Wigner function, or (2) the much more intriguing possibility that the diffusion is successful at decohering the Wigner function, i.e., interference terms are suppressed and the Wigner function is (almost) everywhere positive, yet the late-time distribution is not the solution of the corresponding classical Fokker-Planck equation. We find that the second possibility is the one actually realized, and show how it arises as a consequence of the fact that the classical Fokker-Planck equation violates rho-positivity, while the quantum Master equation does not.

The singular nature of the classical limit $\hbar \to 0$ in quantum mechanics has been appreciated for a long time. However, what has not been stressed sufficiently is the reason for this singular behavior, that classical dynamics violates unitarity and rho-positivity, and thus $\hbar = 0$ cannot be connected smoothly to $\hbar \to 0$. A simple example suffices to make this point clear. Let us consider as initial condition a pure Gaussian state. Let us suppose that we evolve the corresponding (positive) Wigner function classically in some nonlinear potential (for linear systems classical and quantum dynamics are identical [4]), then the distribution becomes no longer Gaussian, but is still positive-definite. Three possibilities now present themselves: the evolved object can be interpreted as (1) a pure quantum state (unitarity is preserved), (2) a mixed quantum state (rho-positivity is preserved), and (3) cannot be interpreted as a quantum state (rho-positivity is violated). The first possibility can be dismissed using Hudson's theorem: the *only* pure state with positive Wigner function is a Gaussian state with a (necessarily) Gaussian Wigner function [5]. But our distribution is non-Gaussian. As to the second, we first note that the phase space integral of any function of the phase space distribution is preserved under a Liouville flow. In particular

$\int f^2(x, p)dxdp$ remains constant. For Wigner functions this quantity is proportional to $Tr\rho^2$ which is a direct measure of whether a state is mixed or not – since this measure cannot change, the evolved object is not interpretable as a mixed state. Thus we are forced to the third alternative, that the evolved object cannot be interpreted as a quantum state at all, i.e., the Weyl transform of the evolved classical distribution yields a 'classical density matrix' which is non-rho-positive [3].

The above analysis makes it clear that the classical Liouville equation can never arise as a formal limit of quantum theory. However, all real experiments deal with open systems, i.e., systems interacting with their environment, of which the particular case of a measuring apparatus (necessary to deduce classical behavior) is an important example. Quantum decoherence and conditioned evolution arising as a consequence of such system-environment couplings and the act of measurement and observation provide a natural pathway to the classical limit as has been quantitatively demonstrated, e.g., in Ref. [6]. Thus, it is important to inquire into the role of rho-positivity violation in this context: When is it important, and when not?

Conditions have been previously derived that apply to the extraction of (noisy) classical trajectories via continuous quantum measurement [6]. Once these (strict) conditions are satisfied (typically in the macroscopic limit $\hbar \ll S$, where S is the system action), measurement induces classical behavior, and in this regime all systems are therefore Type I. However, when these conditions are not satisfied, as is the case in most current experiments, the differences are indeed important. The key point is that, under continuous measurement, Type I systems can violate the classicality conditions in the sense that individual classical trajectories cannot be extracted, yet expectation values are close to the classical results, whereas in Type II systems, violation of the classicality condition also implies a violation of correspondence at the level of expectation values. We will demonstrate this for the QDKR below.

A quantum Master equation representing a weakly coupled, high temperature environment often utilized in studies of decoherence is

$$\frac{\partial}{\partial t} f_W = L_{cl} f_W + L_q f_W + D \frac{\partial^2}{\partial p^2} f_W; \qquad (1)$$

$$L_{cl} \equiv -\frac{p}{m} \frac{\partial}{\partial x} + \frac{\partial V}{\partial x} \frac{\partial}{\partial p}, \qquad (2)$$

$$L_q \equiv \sum_{\lambda \ odd} \frac{1}{\lambda!} \left(\frac{\hbar}{2i}\right)^{\lambda - 1} \frac{\partial^\lambda V(x)}{\partial x^\lambda} \frac{\partial^\lambda}{\partial p^\lambda}. \qquad (3)$$

An unraveling of the weakly-coupled, high temperature environment, Master equation (1) is provided by a continuous measurement of position. This process is described by a stochastic Master equation for the density matrix $\rho(t)$, conditioned on the measurement record $\langle X \rangle + \xi(t)$ with $\xi(t) \equiv (8\eta k)^{-1/2} dW/dt$, [8]

$$\rho(t + dt) = \rho - (\frac{i}{\hbar}[H, \rho] - k[X, [X, \rho]]) \ dt$$
$$+ \sqrt{2\eta k} \ ([X, \rho]_+ - 2\rho \operatorname{Tr} \rho X) \ dW , \qquad (4)$$

where k is a constant specifying the strength of the measurement, η is the measurement efficiency and is a number between 0 and 1, and dW is a Wiener process, satisfying $(dW)^2 = dt$. When $\eta = 1$, the evolution preserves the purity of the state and can be rewritten in a way which allows it to be understood as a series of diffuse projection measurements [9]. Averages over the resulting Schrödinger trajectories reproduce expectation values computed using the reduced density matrix ρ or the corresponding Wigner function $f_W(x, p)$ obtained from solving the Master equation (1). The strength of the measurement is related to the diffusion coefficient of Eq. (1) by $D = \hbar^2 k$.

When the diffusion constant $D = 0$, Eq. (1) is just the quantum Liouville equation for the closed system. Note that the linearity of the quantum Liouville equation implies that in order for the evolution to be unitary, L_q cannot be unitary since L_{cl} is not (the sum $L_{cl} + L_q$ is unitary but not the operators separately). The familiar heuristic argument for obtaining the classical limit from the quantum Master equation is that the diffusion term smooths out the interference effects generated by L_q in such a way that quantum corrections to the classical dynamics are much reduced. It has also been argued, that at finite $\hbar$, the appropriate limiting case of the quantum Master equation is in fact the classical Fokker-Planck equation [setting $L_q = 0$ in Eqn. (1)] rather than the classical Liouville equation [7]. In any case, one immediately appreciates that if *either of the classical equations are strongly rho-positivity-violating, i.e., are Type II* then this implies the existence of compensatory 'large' quantum corrections in the quantum Master equation, and hence the above heuristic argument must fail: L_q is responsible for more than just the generation of interference fringes in the Wigner evolution.

Previous work has already suggested the possibility that closed dynamical systems may be roughly divided into two types depending on the (dynamical) classical-quantum correspondence as follows: (1) Type I systems in which quantum expectation values and classical averages track each other relatively closely as a function of time [7,10], e.g., the driven Duffing oscillator with Hamiltonian,

$$H_{\text{duff}} = p^2/2m + Bx^4 - Ax^2 + \Lambda x \cos(\omega t), \qquad (5)$$

and (2) Type II systems in which the quantum and classical averages diverge sharply after some finite time, e.g., dynamical localization in the QDKR [11]. The QDKR Hamiltonian is

$$H_{\text{dkr}} = \frac{1}{2}p^2 + \kappa \cos q \sum_n \delta(t-n). \tag{6}$$

We solved the classical and quantum Master equations corresponding to Eqs. (5) and (6) using a high-resolution spectral solver implemented on parallel supercomputers. The solver explicitly respects rho-positivity conservation.

We verified that in both the QDKR and the Duffing oscillator numerical examples discussed below the localization condition [6] necessary to obtain classical trajectories was violated. The relevant condition is $8\eta k \gg (\partial_x^2 F/F)\sqrt{\partial_x F/2m}$ where the force F and its derivatives are evaluated at typical points in phase space. For both cases we have in fact, $8\eta k \sim (\partial_x^2 F/F)\sqrt{\partial_x F/2m}$ thus localization does not occur (direct numerical solution of the corresponding stochastic Schrödinger equation confirms this result) and, as discussed earlier, a meaningful distinction between Types I and II is possible. As the value of $\hbar$ is reduced (with D fixed and non-zero) one does expect an approach to the classical limit [6], though the trajectory in the space of D and $\hbar$ need not be simple [12].
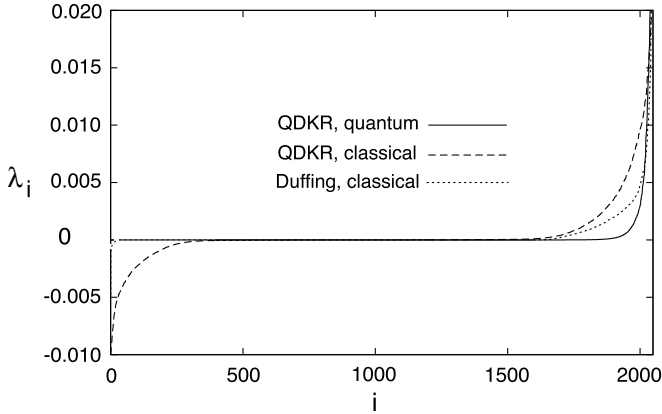

FIG. 1. Eigenvalues of the quantum density matrix (solid) and the classical approximation (long-dashed) computed from the quantum and classical Master equation evolutions for the QDKR at $t = 6$. Also shown (short-dashed) is the classical result for the Duffing oscillator at $t = 10$.

Our numerical code returns us the classical distribution function, the quantum density matrix and the Wigner function as functions of time. We then numerically solve for the eigenvalues of the quantum density matrix and the eigenvalues of the Weyl transform of the classical phase space distribution (the 'classical density matrix'). Results of one such computation are displayed in Fig. 1 for the QDKR (Type II) and Duffing system (Type I). For the QDKR, initial conditions are pure Gaussian Wigner functions characterized by the position width $\Delta x = 2.5$, momentum width $\Delta p = 1$, centered on the point $(x,p) = (0,0)$, and with $\hbar = 5$ and $\kappa = 10$. The diffusion coefficient $D = 0.1$, corresponding to $k = 0.004$. The horizontal axis refers to the index i corresponding to the eigenvalues λ_i, which are themselves plotted on the vertical axis. The solid line is a result from a numerical solution of the quantum Master equation, as expected all eigenvalues are positive (the pure initial state has one eigenvalue equaling unity, the rest being zero). The dashed line is the corresponding result from the classical Fokker-Planck equation, which is characterized by a strong contribution from negative eigenvalues. It is thus clear that the true quantum density matrix and that provided by the classical approximation are in fact quite different. In contrast, results from classical Duffing calculations show a very small contribution from negative eigenvalues [Parameter values in the particular case shown in Fig. 1 were $m = 1$, $A = 10$, $B = 0.5$, $\Lambda = 10$, $\omega = 6.07$, $\Delta x = 0.05$, $\Delta p = 1$, $(x,p) = (-3,8)$, $\hbar = 0.1$, $D = 0.02$.] These results show how rho-positivity violation may be used to distinguish the two types of dynamical systems. An important point to emphasize is that it is sufficient to only carry out the classical dynamical calculation in order to classify a dynamical system as being Type I or II. (The initial condition must of course be a Wigner function.) Also, it should be clear that non-violation of rho-positivity is a necessary but not sufficient condition for quantum-classical correspondence in terms of agreement of expectation values.
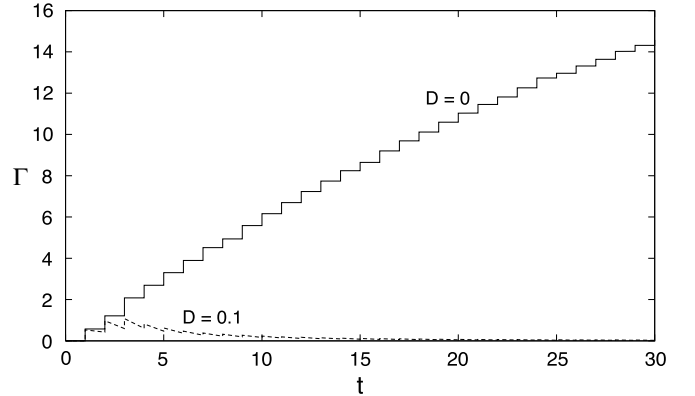

FIG. 2. The Wigner function negativity measure Γ as a function of time for $D = 0$ and $D = 0.1$ for the QDKR.

It is well-known that dynamical localization in the QDKR can be destroyed (in the sense that $\langle p^2(t)\rangle$ no longer saturates at late times) by coupling to external noise or to dissipative channels (e.g., spontaneous emission) [13]. However, what is important to note is that even in the presence of quite strong coupling to these decohering channels, the evolution does not go over to the classical one, and in this sense the QDKR is quite different from the Duffing system investigated in Ref. [7]. In addition to numerically solving the Master equation (1) we have investigated in detail the effects of including amplitude and phase noise, timing jitter in the kicked system, and carried out more realistic simulations taking into account the effects of spontaneous emission. Stability to decoherence in the sense above was manifest in all

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of these cases. Since we have established that the QDKR is a Type II system (Fig. 1), this behavior is essentially forced: as long as the classical evolution strongly violates rho-positivity, it is impossible for the full evolution to ever become close to the classical limit as the quantum corrections must always be concomitantly large. The question remains whether the resulting Wigner function at least has a classical interpretation. In order to investigate this we computed as a function of time, the quantity $\Gamma = \int dx dp (|f_W| - f_W)$, which provides a global measure of negativity of the Wigner function. With $D = 0$, one sees that Γ increases monotonically as the Wigner function develops the expected oscillatory structure as a consequence of quantum interference in phase space. When $D \neq 0$, diffusion in phase space wipes out the interference and produces an essentially positive distribution which one may interpret classically. However, because rho-positivity must be maintained, classical evolution cannot connect two such positive distributions. Thus, in Type II systems decoherence can be successful in rendering the Wigner distribution positive, but yet not lead to a classical limit. We note that in NMR systems there is an interesting question regarding when classical evolution of spins can reproduce quantum evolutions connecting spin states that have no entanglement and thus may be interpreted classically [14]. We have shown that a similar situation can arise even in single-particle evolution where entanglement is not an issue.

Recent experiments have attempted to directly address the issue of environment-induced decoherence in the QDKR, in the context of cold atom optics [1]. Despite some complications stemming from non-ideal realizations, the results indicate that classical and quantum evolutions agree only at inordinately large noise levels. Note that in these experiments, parametric noise or spontaneous emission was used as the decohering mechanism. (The non-selective Master equation for atomic motion in far-detuned laser light has a similar form to that of a particle subjected to continuous position measurement. However, arguments can be made that only the weak decoherence regime can be accessed in this manner.) The parameter values in our numerical work are close to those actually used in the experiments thus, as with our simulations, the experiments are not carried out in a classical regime in the sense of Ref. [6]. And since we have demonstrated the strongly Type II nature of the QDKR, it follows immediately that to observe true classical behavior, either the current experiments have to switch to a Type I system or employ lower values of $\hbar$. Simply increasing the measurement constant k, or equivalently D, while it produces localization, adds noise into the trajectory which must be kept small in order to achieve the classical limit. This final condition requires a reduction in $\hbar$ as k is increased [6].

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